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Curriculum Vitae

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PRESENT POSITION:

Physicist

EDUCATION:

Ph.D., Physics, University of California, Davis, CA, 1989.

RESEARCH INTERESTS:

Atomistic simulations of defect structures in metals and alloys. Computer simulations of classical and quantum systems using molecular dynamics and quantum molecular dynamics methods. Electronic and structural properties of metals and alloys. Algorithm development on massively parallel processor platforms.

RESEARCH DIRECTIONS:

- Electron transport in materials using quantum molecular dynamics simulations
- Electronic properties of device materials, semiconductor superlattices, and metal-semiconductor interfaces.
- Large-scale *ab initio* calculations of transition metal surfaces, defects and dopants in semiconductors.
- Structural and thermodynamical properties of point defects in metals and alloys.
- Atomistic simulations of misfit-defect structures and solute segregation at ceramic/metal interfaces, including potential fittings from *ab initio* calculations.
- Atomistic simulations of dislocation process in metals and alloys.
- Quantum and atomistic simulations of stress corrosion cracking in metals and alloys.
- Algorithm development for large-scale computer simulations on parallel architectures.
- Large-scale computing on peta- to peta-scale platforms.

PROFESSIONAL EMPLOYMENTS:

Oct.(1988)–Jan.(1991), Postdoc, Argonne National Laboratory, IL.
Oct.(1991)–Jan.(1993), Postdoc, Lawrence Livermore National Laboratory, CA.
Feb.(1991)–Present, Physicist, Lawrence Livermore National Laboratory, CA.

PROFESSIONAL AFFILIATIONS:

- The American Physical Society.
- The Materials Research Society.
- Member-at-Large, American Physical Society California Section, 2006-present.

PUBLICATIONS:

1. The Doping Mechanism in Amorphous Silicon, C. S. Nichols, L. H. Yang, and C. Y. Fong, J. Non-Cryst. Sol. **97** & **98**, 495 (1987)
2. Localization of Multivibrational Excitations, M. S. Wartak, L. H. Yang, C. Y. Fong, and Y. R. Shen, Phys. Rev. B **37**, 10350 (1988).
3. Electronic Properties of Si-Ge Micro NIPI Structure, L. H. Yang, C. Y. Fong, and J. S. Nelson, " Heteroepitaxy on Silicon: Fundamentals, Structures, and Devices", eds H. K. Choi, R. Hull, H. Ishiwara, and R. J. Newmanich (MRS, Pittsburgh, 1988), p.513.
4. Impurity State-Dangling Bond Pairs in Hydrogenated Amorphous Silicon, L. H. Yang, C. Y. Fong, and C. S. Nichols, "Amorphous Silicon Technology", eds . Y. Hamakawa, P.G. LeComber, A. Madan, P. C. Taylor, and M. J. Thompson (MRS, Pittsburgh, 1988), p.513.
5. A Theoretical Study of Na Overlays on the GaAs(110) Surface, C. Y. Fong, L. H. Yang, and Inder P. Batra," Metallization and Metal-Semiconductor Interfaces", ed. Inder P. Batra (Plenum, New York, 1989), p.449.
6. Electronic Properties of Micro *n-i-p-i* Structures in Silicon Superlattices, L. H. Yang, R. F. Gallup, C. Y. Fong, and J. S. Nelson, Phys. Rev. B **39**, 3795 (1989)
7. Electronic Properties of Na Overlays on the GaAs(110) Surface, C. Y. Fong, L. H. Yang, and Inder P. Batra, Phys. Rev. B **40**, 6120 (1989)

8. Electronic Properties of the Donor States Under Two-dimensional-conductor and Quantum-wire Configurations in Heavily and Orderly Doped (GaAs)-(AlAs), C. Y. Fong, L. H. Yang, J. S. Nelson, and L. Esaki, Phys. Rev. B**41**, 10667 (1990).
9. Compensated Dopants in Hydrogenated Amorphous Silicon, L. H. Yang and C. Y. Fong, "Amorphous Silicon Technology", eds Y. Hamakawa, P. G. LeComber, A. Madan, P. C. Taylor, and M. J. Thompson (MRS, Pittsburgh, 1989), Vol. 191, p445.
10. Quantum Molecular Dynamics - A New Algorithm for Linear and Nonlinear Electron Transport in Disordered Materials, R. K. Kalia, P. Vashishta, L. H. Yang, F. Dech, and J. Rowlan, The Inter. J. Supercom. App. **4**, 22 (1990).
11. Electron Trapping in Amorphous Silicon - A Quantum Molecular Dynamics Study, L. H. Yang, R.K. Kalia, and P. Vashishta, "Amorphous Silicon Technology", eds Y. Hamakawa, P. G. LeComber, A. Madan, P. C. Taylor, and M. J. Thompson (MRS, Pittsburgh, 1990), Vol. 192, p781.
12. Impurity-Defect Complexes in Hydrogenated Amorphous Silicon, L. H. Yang, C. Y. Fong, and C. S. Nichols, "Amorphous Silicon Technology", eds Y. Hamakawa, P. G. LeComber, A. Madan, P. C. Taylor, and M. J. Thompson (MRS, Pittsburgh, 1991).
13. Impurity-Defect Complexes and Doping Mechanism in Hydrogenated Amorphous Silicon, L. H. Yang, C. Y. Fong, and C. S. Nichols, Phys. Rev. Lett. **66**, 3273 (1991).
14. Formation Energy and Lattice-Relaxation for Point Defects in Li and Al, R. Benedek, L.H.Yang, C. Woodward, and B.I. Min, Phys. Rev. B**45**, 2607 (1992).
15. Probing Excess Electron Localization and Mobility in Amorphous Silicon by Quantum Molecular Dynamics Method, A. Nakano, P. Vashishta, R. K. Kalia, and L. H. Yang, Phys. Rev. B**45**, 8363 (1992).
16. Possible Doping Mechanism in Hydrogenated Amorphous Silicon — an Impurity-Defect Complex Model, C. Y. Fong and L. H. Yang, Mod. Phys. Letts. B**6**, 235 (1992).
17. Polymeric Nitrogen, C. Mailhot, L. H. Yang, and A. K. McMahan, Phys. Rev. B**46**, 14419 (1992-II).
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19. A Link-Cell Domain Decomposition Method for Molecular Dynamics Simulation on a Scalable Multiprocessor, L. H. Yang, E. D. Brooks III, and J. Belak, Scientific Programming **1**, 153 (1993).

20. Bonding Properties of the Interacting Donor and Acceptor States of Si-doped *n-i-p-i* Structures in GaAs, C. Y. Fong, J. S. Nelson, and L. H. Yang, Modeling and Simul. Mater. Sci. and Eng. **1**, 349 (1993).
21. Effect of Semicore Banding on Heavy Alkali Metal Lattice Constants: Beyond the Frozen-Core Approximation, L. H. Yang, A. P. Smith, and R. Benedek, Phys. Rev. **B47**, 16101 (1993).
22. The Insulator-Metal Transition in Expanded Cesium, M. Ross, L. H. Yang, B. Dahling and N. Winter, Zeitschrift Für Physikalische Chemie, Bd. 184, S.65 (1994).
23. Polymeric nitrogen, C. Mailhiot, L. H. Yang, A. K. McMahan, and T. W. Barbee III, AIP Conference Proceedings, **309**, 221 (1994).
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26. Atomic Potentials for Rb- and K- Graphite Intercalation Compounds, R. Benedek, A. P. Smith, and L. H. Yang, Phys. Rev. **B49**, 5050 (1994).
27. Band Discontinuities at Heterojunctions between Crystalline and Amorphous Silicon, C.G. Van de Walle and L.H. Yang, J. Vac. Sci. & Tech. **B13**, 1635 (1995).
28. *Ab-initio* Pseudopotential Calculations of Point Defects and Boron Impurity in Silicon, J. Zhu, L.H. Yang, C. Mailhiot, T. Dias de la Rubia, and G. Gilmer , Nuclear Instruments and Methods in Physics Research, **B102**, 29 (1995).
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